



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:31 pm BST

PDB ID : 1K74
Title : The 2.3 Angstrom resolution crystal structure of the heterodimer of the human PPARgamma and RXRalpha ligand binding domains respectively bound with GW409544 and 9-cis retinoic acid and co-activator peptides.
Authors : Xu, H.E.; Lambert, M.H.; Montana, V.G.; Moore, L.B.; Collins, J.L.; Oplinger, J.A.; Kliewer, S.A.; Gampe Jr., R.T.; McKee, D.D.; Moore, J.T.; Willson, T.M.
Deposited on : 2001-10-18
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

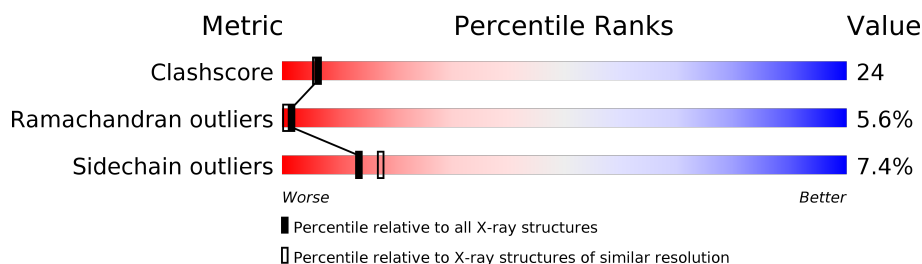
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	238	<div> <div>63%</div> <div>29%</div> <div>5%</div> <div>••</div> </div>
2	D	283	<div> <div>58%</div> <div>32%</div> <div>5%</div> <div>••</div> </div>
3	B	25	<div> <div>24%</div> <div>16%</div> <div>60%</div> </div>
3	E	25	<div> <div>28%</div> <div>36%</div> <div>36%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	544	D	478	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4405 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1754	1117	306	321	10			

- Molecule 2 is a protein called Peroxisome proliferator activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	272	Total	C	N	O	S	0	0	0
			2168	1399	354	405	10			

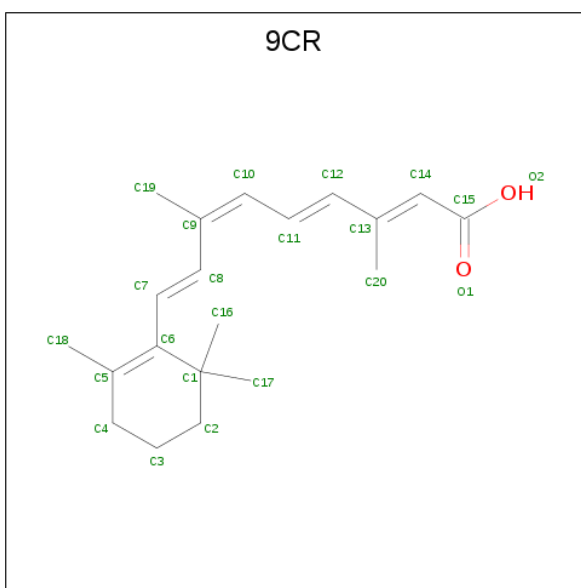
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	195	MET	-	EXPRESSION TAG	UNP P37231
D	196	LYS	-	EXPRESSION TAG	UNP P37231
D	197	LYS	-	EXPRESSION TAG	UNP P37231
D	198	GLY	-	EXPRESSION TAG	UNP P37231
D	199	HIS	-	EXPRESSION TAG	UNP P37231
D	200	HIS	-	EXPRESSION TAG	UNP P37231
D	201	HIS	-	EXPRESSION TAG	UNP P37231
D	202	HIS	-	EXPRESSION TAG	UNP P37231
D	203	HIS	-	EXPRESSION TAG	UNP P37231
D	204	HIS	-	EXPRESSION TAG	UNP P37231
D	205	GLY	-	EXPRESSION TAG	UNP P37231

- Molecule 3 is a protein called steroid receptor coactivator.

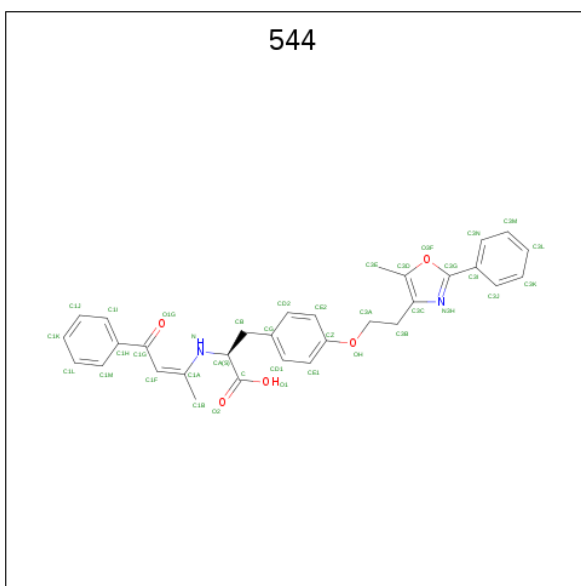
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	10	Total	C	N	O	0	0	0
			86	55	18	13			
3	E	16	Total	C	N	O	0	0	0
			129	79	27	23			

- Molecule 4 is (9cis)-retinoic acid (three-letter code: 9CR) (formula: $C_{20}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			22	20	2		

- Molecule 5 is 2-(1-METHYL-3-OXO-3-PHENYL-PROPYLAMINO)-3-{4-[2-(5-METHYL-2-PHENYL-OXAZOL-4-YL)-ETHOXY]-PHENYL}-PROPIONIC ACID (three-letter code: 544) (formula: $C_{31}H_{30}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			38	31	2	5		

- Molecule 6 is water.

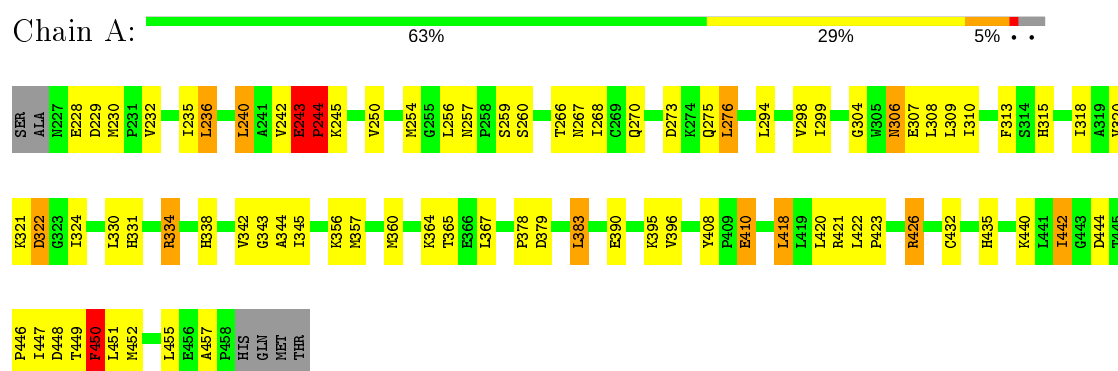
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	67	Total 67	O 67	0	0
6	D	133	Total 133	O 133	0	0
6	B	2	Total 2	O 2	0	0
6	E	6	Total 6	O 6	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: Retinoic acid receptor RXR-alpha



CYS	PRO	SER	SER	HIS	SER	SER	LEU	THR	E685	R686	H687	K688	I689	L690	H691	R692	L693	L694	Q695	E696	G697	S698	P699	S700
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.62Å 55.10Å 214.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.238 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4405	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 9CR, 544

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.36	0/1789	0.62	2/2414 (0.1%)
2	D	0.41	0/2206	0.66	1/2974 (0.0%)
3	B	0.31	0/87	0.62	0/116
3	E	0.29	0/131	0.51	0/175
All	All	0.39	0/4213	0.64	3/5679 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	GLU	C-N-CD	-10.50	97.50	120.60
1	A	243	GLU	C-N-CA	6.57	149.59	122.00
2	D	206	PRO	N-CA-CB	5.53	109.94	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1754	0	1733	73	0
2	D	2168	0	2213	126	1
3	B	86	0	86	5	0
3	E	129	0	125	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	22	0	27	7	0
5	D	38	0	29	1	0
6	A	67	0	0	0	0
6	B	2	0	0	1	0
6	D	133	0	0	2	0
6	E	6	0	0	2	0
All	All	4405	0	4213	203	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:270:LEU:HD12	2:D:270:LEU:H	1.19	1.05
2:D:270:LEU:HD22	2:D:283:GLN:HB3	1.37	1.05
1:A:230:MET:HE3	1:A:235:ILE:HD11	1.38	1.05
2:D:268:THR:H	2:D:269:PRO:HD2	1.26	1.00
2:D:270:LEU:CD1	2:D:270:LEU:H	1.83	0.89
2:D:273:GLN:O	2:D:275:LYS:N	2.06	0.89
2:D:270:LEU:HD22	2:D:283:GLN:CB	2.05	0.86
2:D:270:LEU:CD1	2:D:284:GLY:HA2	2.07	0.85
1:A:230:MET:CE	1:A:235:ILE:HD11	2.06	0.85
2:D:270:LEU:HD21	2:D:283:GLN:O	1.77	0.85
1:A:229:ASP:HB3	1:A:395:LYS:HD3	1.59	0.84
2:D:270:LEU:CD2	2:D:283:GLN:HB3	2.07	0.83
2:D:471:GLU:OE1	3:E:689:ILE:HG22	1.79	0.83
2:D:358:LYS:HB2	2:D:359:PRO:HD2	1.61	0.83
2:D:270:LEU:HD11	2:D:284:GLY:HA2	1.62	0.82
4:A:463:9CR:H8	4:A:463:9CR:H19	1.61	0.81
2:D:258:GLY:O	2:D:260:ASP:N	2.12	0.81
2:D:335:ASN:C	2:D:335:ASN:HD22	1.85	0.80
2:D:262:ILE:H	2:D:269:PRO:CG	1.95	0.80
2:D:466:HIS:HD2	2:D:468:LEU:H	1.31	0.78
2:D:262:ILE:CB	2:D:272:GLU:HG2	2.15	0.77
1:A:449:THR:HG22	3:B:632:ILE:HD11	1.66	0.76
2:D:270:LEU:N	2:D:270:LEU:HD12	2.00	0.76
1:A:423:PRO:HG3	2:D:440:THR:HG22	1.69	0.75
1:A:426:ARG:HH11	1:A:426:ARG:HB2	1.50	0.74
1:A:298:VAL:HG13	3:B:633:LEU:HD12	1.71	0.73
2:D:277:VAL:O	2:D:280:ARG:HB2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:262:ILE:O	2:D:263:LYS:HG2	1.88	0.73
2:D:358:LYS:CB	2:D:359:PRO:CD	2.67	0.72
1:A:320:VAL:HG21	1:A:331:HIS:CE1	2.26	0.71
2:D:271:GLN:CB	2:D:280:ARG:HD2	2.21	0.70
2:D:262:ILE:H	2:D:269:PRO:HG2	1.58	0.69
2:D:456:ILE:HG22	2:D:463:MET:HG2	1.75	0.69
2:D:250:TYR:O	2:D:352:PHE:HB2	1.92	0.69
1:A:426:ARG:NH1	1:A:426:ARG:HB2	2.08	0.68
1:A:236:LEU:HD22	1:A:240:LEU:HD22	1.75	0.67
2:D:262:ILE:H	2:D:269:PRO:HG3	1.58	0.67
2:D:262:ILE:N	2:D:269:PRO:HG2	2.10	0.67
2:D:358:LYS:HB2	2:D:359:PRO:CD	2.23	0.67
2:D:335:ASN:ND2	2:D:337:ASP:H	1.95	0.65
1:A:310:ILE:HA	1:A:313:PHE:CE2	2.32	0.65
1:A:338:HIS:CD2	1:A:343:GLY:HA3	2.33	0.64
2:D:276:GLU:O	2:D:279:ILE:HG22	1.99	0.63
1:A:451:LEU:O	1:A:455:LEU:HD13	1.99	0.63
2:D:250:TYR:HB2	2:D:349:THR:CG2	2.30	0.62
3:E:685:GLU:HB2	3:E:687:HIS:CE1	2.33	0.62
2:D:262:ILE:N	2:D:269:PRO:CG	2.63	0.62
1:A:228:GLU:O	1:A:228:GLU:HG3	2.00	0.61
1:A:268:ILE:HG21	4:A:463:9CR:H21	1.82	0.61
2:D:476:LEU:HG	2:D:477:TYR:HD1	1.67	0.60
2:D:268:THR:N	2:D:269:PRO:HD2	2.04	0.60
2:D:325:ILE:HD13	2:D:388:ILE:HG23	1.82	0.60
2:D:242:THR:O	2:D:243:ASP:HB3	2.01	0.59
2:D:343:GLU:HB2	2:D:345:GLN:HE21	1.67	0.59
2:D:411:ASP:HB3	6:D:568:HOH:O	2.01	0.59
2:D:271:GLN:C	2:D:280:ARG:CD	2.71	0.59
2:D:235:ALA:O	2:D:241:THR:HG22	2.02	0.59
1:A:268:ILE:HG21	4:A:463:9CR:C18	2.33	0.58
2:D:466:HIS:CD2	2:D:468:LEU:H	2.19	0.58
2:D:383:ASP:OD2	2:D:425:HIS:HE1	1.86	0.58
2:D:270:LEU:HD13	2:D:284:GLY:HA2	1.85	0.58
1:A:243:GLU:HB2	1:A:244:PRO:O	2.03	0.58
2:D:286:GLN:HG2	2:D:469:LEU:HD12	1.85	0.58
2:D:250:TYR:HB2	2:D:349:THR:HG21	1.86	0.58
2:D:357:ARG:NH1	2:D:358:LYS:HB2	2.19	0.57
2:D:476:LEU:HG	2:D:477:TYR:CD1	2.39	0.57
1:A:379:ASP:OD1	2:D:373:LYS:HE2	2.04	0.57
2:D:271:GLN:CB	2:D:283:GLN:OE1	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:PRO:CG	2:D:440:THR:HG22	2.35	0.56
2:D:286:GLN:CG	2:D:469:LEU:HD12	2.36	0.56
1:A:230:MET:CE	1:A:396:VAL:HG22	2.36	0.56
2:D:468:LEU:O	2:D:472:ILE:HG13	2.06	0.56
2:D:271:GLN:CB	2:D:280:ARG:CD	2.83	0.55
1:A:298:VAL:HA	3:B:633:LEU:HD11	1.87	0.55
3:E:689:ILE:HD11	6:E:142:HOH:O	2.06	0.55
1:A:338:HIS:HD2	1:A:343:GLY:HA3	1.70	0.55
1:A:447:ILE:HD12	1:A:451:LEU:HG	1.89	0.55
2:D:335:ASN:ND2	2:D:338:GLY:H	2.04	0.55
2:D:271:GLN:C	2:D:280:ARG:HD3	2.27	0.54
1:A:378:PRO:HG3	1:A:390:GLU:OE1	2.07	0.53
2:D:457:LYS:HA	2:D:463:MET:HG3	1.89	0.53
1:A:268:ILE:HD13	4:A:463:9CR:H21	1.90	0.53
2:D:271:GLN:CB	2:D:280:ARG:NE	2.71	0.53
3:E:685:GLU:HG2	3:E:686:ARG:H	1.74	0.52
1:A:356:LYS:HG3	1:A:421:ARG:NH1	2.25	0.52
2:D:260:ASP:CG	2:D:265:LYS:NZ	2.63	0.52
2:D:260:ASP:HA	2:D:265:LYS:HE3	1.90	0.52
1:A:320:VAL:HG22	1:A:321:LYS:N	2.25	0.51
2:D:357:ARG:HG3	2:D:357:ARG:HH11	1.73	0.51
2:D:443:ARG:O	2:D:447:THR:HG23	2.11	0.51
1:A:228:GLU:O	1:A:229:ASP:HB2	2.10	0.51
1:A:343:GLY:O	1:A:344:ALA:HB3	2.08	0.51
2:D:358:LYS:CB	2:D:359:PRO:HD2	2.33	0.51
1:A:408:TYR:HA	1:A:410:GLU:OE2	2.10	0.51
1:A:449:THR:O	1:A:450:PHE:CB	2.58	0.51
2:D:253:ASN:OD1	2:D:257:MET:CE	2.59	0.51
2:D:471:GLU:CG	3:E:687:HIS:HA	2.41	0.50
1:A:276:LEU:HB3	1:A:450:PHE:CE1	2.46	0.50
2:D:291:GLU:O	2:D:295:GLU:HG3	2.11	0.50
2:D:330:LEU:O	2:D:334:MET:HG3	2.11	0.50
1:A:230:MET:HE2	1:A:396:VAL:HG22	1.92	0.50
2:D:270:LEU:N	2:D:270:LEU:CD1	2.55	0.49
2:D:468:LEU:HD13	3:E:689:ILE:CG2	2.41	0.49
2:D:224:LYS:HE2	6:D:606:HOH:O	2.12	0.49
1:A:447:ILE:HD11	1:A:452:MET:SD	2.53	0.49
2:D:358:LYS:HB3	2:D:359:PRO:CD	2.41	0.49
1:A:449:THR:HG22	3:B:632:ILE:CD1	2.40	0.49
1:A:266:THR:O	1:A:270:GLN:HG3	2.12	0.49
2:D:268:THR:H	2:D:269:PRO:CD	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:286:GLN:OE1	2:D:466:HIS:N	2.37	0.49
2:D:342:SER:O	2:D:345:GLN:HG3	2.13	0.49
1:A:307:GLU:OE1	1:A:426:ARG:NH1	2.46	0.48
3:E:685:GLU:O	3:E:686:ARG:HB3	2.13	0.48
2:D:335:ASN:C	2:D:335:ASN:ND2	2.57	0.48
1:A:276:LEU:HD13	1:A:309:LEU:HD21	1.94	0.48
2:D:280:ARG:NE	2:D:280:ARG:HA	2.28	0.48
2:D:271:GLN:CB	2:D:280:ARG:HE	2.27	0.48
3:E:693:LEU:HD23	3:E:697:GLY:O	2.13	0.48
1:A:275:GLN:HG3	4:A:463:9CR:O1	2.13	0.48
1:A:315:HIS:CG	1:A:367:LEU:HD22	2.49	0.47
2:D:260:ASP:O	2:D:260:ASP:OD2	2.32	0.47
1:A:304:GLY:O	1:A:308:LEU:HG	2.14	0.47
1:A:273:ASP:OD1	1:A:449:THR:O	2.33	0.47
2:D:237:LEU:HD11	2:D:340:LEU:HG	1.96	0.47
1:A:276:LEU:HA	1:A:276:LEU:HD12	1.78	0.47
2:D:403:VAL:HG12	2:D:407:GLU:HG3	1.97	0.47
1:A:435:HIS:HB2	4:A:463:9CR:H17	1.97	0.47
2:D:275:LYS:CB	2:D:275:LYS:NZ	2.78	0.47
2:D:239:GLY:O	2:D:240:LYS:HD3	2.15	0.47
1:A:440:LYS:C	1:A:442:ILE:H	2.18	0.46
1:A:313:PHE:CE1	1:A:324:ILE:HD13	2.51	0.46
1:A:243:GLU:OE1	1:A:364:LYS:NZ	2.49	0.46
2:D:451:GLN:O	2:D:454:GLN:HB2	2.15	0.46
2:D:468:LEU:HD13	3:E:689:ILE:HG23	1.97	0.46
1:A:243:GLU:CB	1:A:244:PRO:C	2.84	0.46
2:D:447:THR:O	2:D:451:GLN:HG3	2.16	0.46
2:D:288:ARG:HD2	2:D:288:ARG:HA	1.78	0.46
1:A:306:ASN:H	1:A:306:ASN:HD22	1.64	0.46
2:D:261:LYS:O	2:D:262:ILE:CB	2.63	0.46
2:D:474:LYS:HE2	6:E:109:HOH:O	2.16	0.45
1:A:236:LEU:HG	1:A:365:THR:OG1	2.16	0.45
2:D:259:GLU:CB	2:D:263:LYS:HB2	2.46	0.45
1:A:423:PRO:CD	2:D:440:THR:HG22	2.46	0.45
2:D:471:GLU:HG3	3:E:687:HIS:HA	1.97	0.45
2:D:261:LYS:HA	2:D:269:PRO:HG3	1.98	0.45
2:D:275:LYS:O	2:D:276:GLU:HB2	2.16	0.45
2:D:363:PHE:CE2	2:D:456:ILE:HD11	2.51	0.45
2:D:468:LEU:HB2	3:E:689:ILE:HD13	1.99	0.45
1:A:318:ILE:HD11	1:A:357:MET:HB3	1.98	0.45
2:D:360:PHE:HD1	5:D:478:544:H1L1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ASP:CG	1:A:448:ASP:HB2	2.38	0.44
2:D:286:GLN:OE1	2:D:465:LEU:HA	2.17	0.44
1:A:321:LYS:O	1:A:322:ASP:C	2.56	0.44
1:A:330:LEU:HD23	1:A:331:HIS:N	2.33	0.44
2:D:275:LYS:HB3	2:D:275:LYS:NZ	2.33	0.44
2:D:290:VAL:O	2:D:294:GLN:HG3	2.18	0.44
1:A:360:MET:HE1	1:A:418:LEU:HD13	1.99	0.44
1:A:342:VAL:C	1:A:343:GLY:O	2.54	0.44
2:D:471:GLU:CD	3:E:689:ILE:HG22	2.38	0.43
3:E:685:GLU:N	3:E:685:GLU:OE1	2.51	0.43
2:D:238:THR:O	2:D:240:LYS:HE2	2.18	0.43
2:D:270:LEU:CD2	2:D:283:GLN:C	2.87	0.43
2:D:358:LYS:HB3	2:D:359:PRO:HD3	2.00	0.43
1:A:243:GLU:HB3	1:A:244:PRO:C	2.39	0.43
1:A:267:ASN:HD22	1:A:330:LEU:CD1	2.31	0.43
1:A:276:LEU:HB3	1:A:450:PHE:CD1	2.54	0.43
3:B:635:ARG:CZ	6:B:174:HOH:O	2.66	0.43
1:A:299:ILE:HG21	1:A:383:LEU:HD13	2.01	0.43
2:D:357:ARG:NH1	2:D:358:LYS:CG	2.81	0.43
2:D:237:LEU:HD13	2:D:340:LEU:HD21	2.00	0.42
2:D:292:ALA:O	2:D:296:ILE:HG13	2.19	0.42
2:D:341:ILE:O	2:D:341:ILE:HG13	2.17	0.42
1:A:228:GLU:O	1:A:229:ASP:CB	2.67	0.42
1:A:306:ASN:H	1:A:306:ASN:ND2	2.17	0.42
1:A:242:VAL:O	1:A:242:VAL:HG23	2.20	0.42
2:D:250:TYR:CB	2:D:349:THR:CG2	2.96	0.42
2:D:357:ARG:HH11	2:D:358:LYS:CG	2.32	0.42
1:A:426:ARG:CB	1:A:426:ARG:HH11	2.26	0.42
1:A:432:CYS:SG	4:A:463:9CR:H18	2.60	0.42
2:D:377:LEU:CB	2:D:379:LEU:CD1	2.98	0.42
1:A:420:LEU:HD23	1:A:420:LEU:HA	1.82	0.41
2:D:242:THR:HG23	2:D:242:THR:O	2.20	0.41
2:D:271:GLN:O	2:D:280:ARG:CZ	2.68	0.41
2:D:379:LEU:HD21	2:D:435:LEU:HD13	2.01	0.41
1:A:306:ASN:O	1:A:310:ILE:HG13	2.19	0.41
2:D:272:GLU:O	2:D:274:SER:N	2.53	0.41
2:D:286:GLN:HG2	2:D:469:LEU:CD1	2.50	0.41
2:D:335:ASN:ND2	2:D:337:ASP:N	2.63	0.41
3:E:687:HIS:O	3:E:691:HIS:HD2	2.04	0.41
1:A:267:ASN:HB3	1:A:330:LEU:HD13	2.03	0.41
1:A:243:GLU:CD	1:A:364:LYS:NZ	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:357:ARG:HG3	2:D:357:ARG:NH1	2.36	0.41
2:D:325:ILE:HD11	2:D:392:ILE:HG13	2.02	0.41
2:D:365:GLU:HB3	2:D:366:PRO:HD3	2.03	0.41
2:D:411:ASP:O	2:D:415:GLN:HG3	2.20	0.41
2:D:397:ARG:HA	2:D:398:PRO:HD3	1.97	0.41
2:D:293:VAL:HG22	2:D:322:VAL:HG11	2.02	0.41
2:D:357:ARG:HH11	2:D:358:LYS:HB2	1.83	0.41
2:D:377:LEU:HB2	2:D:379:LEU:CD1	2.51	0.41
1:A:334:ARG:HH11	1:A:338:HIS:HE1	1.68	0.40
2:D:262:ILE:CB	2:D:272:GLU:CG	2.93	0.40
1:A:294:LEU:C	1:A:294:LEU:HD23	2.42	0.40
1:A:422:LEU:HB2	2:D:440:THR:HG21	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:250:TYR:OH	2:D:269:PRO:O[4_455]	2.03	0.17

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/238 (97%)	194 (84%)	21 (9%)	15 (6%)	1	0
2	D	270/283 (95%)	242 (90%)	16 (6%)	12 (4%)	2	1
3	B	8/25 (32%)	6 (75%)	1 (12%)	1 (12%)	0	0
3	E	14/25 (56%)	10 (71%)	3 (21%)	1 (7%)	1	0
All	All	522/571 (91%)	452 (87%)	41 (8%)	29 (6%)	2	1

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	GLU
1	A	244	PRO
1	A	256	LEU
1	A	257	ASN
1	A	259	SER
1	A	260	SER
1	A	446	PRO
1	A	450	PHE
2	D	243	ASP
2	D	259	GLU
2	D	267	ILE
2	D	274	SER
2	D	358	LYS
1	A	245	LYS
1	A	250	VAL
2	D	262	ILE
2	D	265	LYS
2	D	271	GLN
2	D	464	SER
1	A	254	MET
2	D	244	LYS
1	A	322	ASP
1	A	442	ILE
2	D	268	THR
2	D	280	ARG
3	B	631	LYS
3	E	699	PRO
1	A	444	ASP
1	A	457	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/205 (89%)	169 (93%)	13 (7%)	14	19
2	D	240/254 (94%)	221 (92%)	19 (8%)	12	15
3	B	9/24 (38%)	9 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	14/24 (58%)	13 (93%)	1 (7%)	14	19
All	All	445/507 (88%)	412 (93%)	33 (7%)	13	17

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	VAL
1	A	236	LEU
1	A	240	LEU
1	A	244	PRO
1	A	276	LEU
1	A	306	ASN
1	A	334	ARG
1	A	345	ILE
1	A	383	LEU
1	A	410	GLU
1	A	418	LEU
1	A	426	ARG
1	A	450	PHE
2	D	207	GLU
2	D	216	LYS
2	D	228	LEU
2	D	237	LEU
2	D	241	THR
2	D	251	ASP
2	D	252	MET
2	D	270	LEU
2	D	274	SER
2	D	276	GLU
2	D	280	ARG
2	D	289	SER
2	D	318	LEU
2	D	335	ASN
2	D	424	ASN
2	D	440	THR
2	D	442	LEU
2	D	463	MET
2	D	477	TYR
3	E	695	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	270	GLN
1	A	275	GLN
1	A	306	ASN
1	A	331	HIS
1	A	338	HIS
2	D	273	GLN
2	D	308	ASN
2	D	335	ASN
2	D	345	GLN
2	D	375	ASN
2	D	415	GLN
2	D	424	ASN
2	D	425	HIS
2	D	454	GLN
2	D	466	HIS
3	B	638	GLN
3	E	691	HIS
3	E	695	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	544	D	478	-	34,41,41	2.75	16 (47%)	39,55,55	1.43	2 (5%)
4	9CR	A	463	-	19,22,22	3.89	11 (57%)	26,30,30	1.90	7 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	9CR	A	463	-	-	4/13/32/32	0/1/1/1
5	544	D	478	-	1/1/4/6	1/23/30/30	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	463	9CR	C1-C6	10.11	1.67	1.53
4	A	463	9CR	C5-C6	9.58	1.51	1.34
5	D	478	544	C1A-N	8.25	1.44	1.33
5	D	478	544	C3E-C3D	4.60	1.54	1.48
5	D	478	544	C1F-C1G	4.57	1.58	1.43
5	D	478	544	CA-N	4.53	1.52	1.46
5	D	478	544	CE2-CZ	3.83	1.46	1.38
4	A	463	9CR	C20-C13	3.70	1.58	1.50
4	A	463	9CR	C14-C13	3.67	1.39	1.35
5	D	478	544	C1I-C1H	3.52	1.45	1.39
4	A	463	9CR	C10-C9	3.29	1.40	1.35
5	D	478	544	C1H-C1G	-3.20	1.44	1.49
4	A	463	9CR	C4-C5	3.16	1.57	1.51
4	A	463	9CR	C2-C1	3.00	1.61	1.54
5	D	478	544	CB-CA	2.87	1.57	1.53
4	A	463	9CR	C12-C13	-2.82	1.39	1.45
5	D	478	544	CD1-CG	2.71	1.44	1.38
5	D	478	544	C3G-N3H	2.68	1.42	1.35
5	D	478	544	C1M-C1H	2.61	1.43	1.39
5	D	478	544	C3N-C3I	2.61	1.44	1.39
4	A	463	9CR	C16-C1	2.53	1.58	1.53
4	A	463	9CR	C2-C3	2.46	1.58	1.52
5	D	478	544	CD2-CG	2.28	1.43	1.38
5	D	478	544	OH-CZ	2.14	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	478	544	CE1-CD1	2.14	1.42	1.38
5	D	478	544	C1L-C1K	2.10	1.43	1.38
4	A	463	9CR	C11-C10	-2.06	1.37	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	478	544	C1F-C1A-N	-5.17	117.16	121.29
5	D	478	544	C1B-C1A-N	5.07	124.50	118.82
4	A	463	9CR	C19-C9-C10	-4.56	116.53	122.92
4	A	463	9CR	C19-C9-C8	3.46	123.52	118.08
4	A	463	9CR	C20-C13-C12	3.36	123.37	118.08
4	A	463	9CR	C1-C6-C5	-3.09	118.26	122.61
4	A	463	9CR	C2-C1-C6	2.85	114.88	110.48
4	A	463	9CR	C17-C1-C6	2.51	114.37	110.30
4	A	463	9CR	C7-C8-C9	2.46	129.95	126.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	478	544	C1A

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	463	9CR	C1-C6-C7-C8
4	A	463	9CR	C5-C6-C7-C8
5	D	478	544	C-CA-N-C1A
4	A	463	9CR	C11-C10-C9-C19
4	A	463	9CR	C11-C10-C9-C8

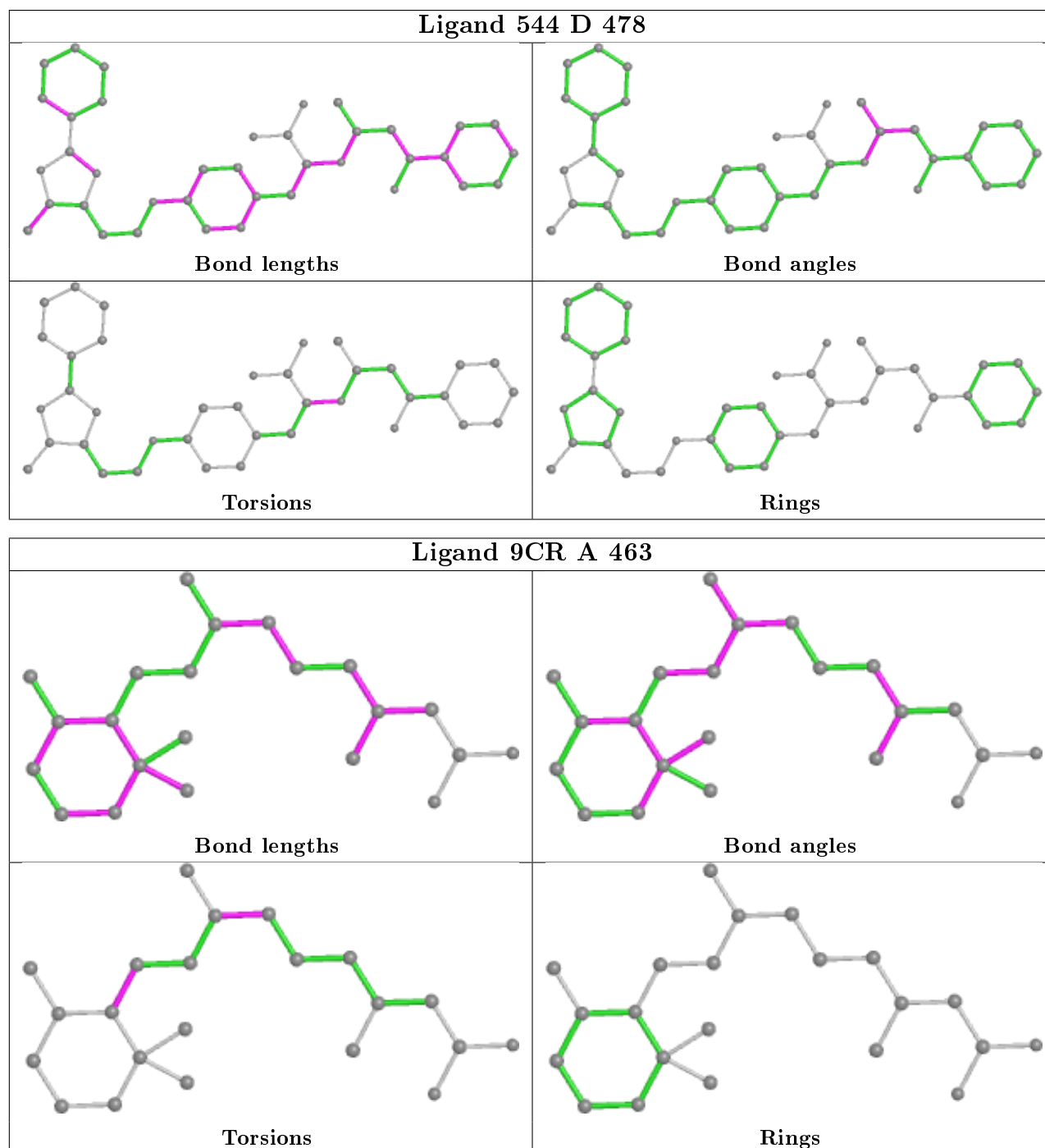
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	478	544	1	0
4	A	463	9CR	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.